Charge Configuration and its effect on Permeation through Carbon Nanotube

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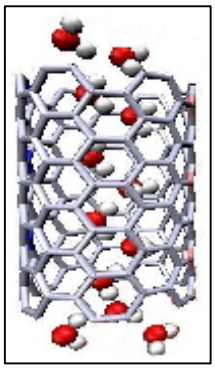
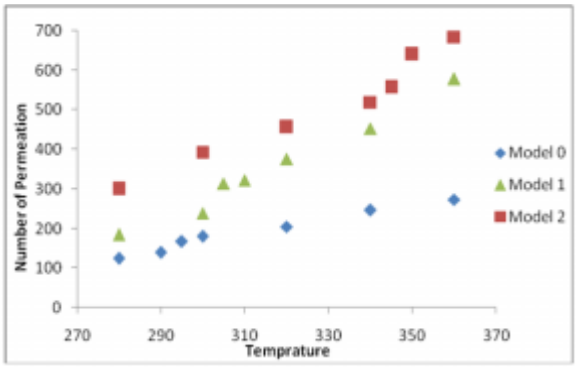
In order to investigate the mechanism of water permeation through modified CNTs, we applied charge distributions on CNTs wall which are in accordance with the proposed biological as well as channel membranes [1]. We have carried out two simulations for each system, one without induced pressure difference to find out the diffusion permeation (p_d) and the other with induced pressure difference (p_f) to obtain the osmotic permeation.

We build tree kind of channels based on the configuration of proposed artificial Ion Channels[2], one prototype CNT – denotes as model 0- and two modified ones. One is the modified CNTs with three positive and three negative charges on two sides of CNTs wall and positives on one side and negatives on the other side along *z*-direction, denoted as model1. The other one, model2 consists of modified CNTs with three charges on each side of CNT wall with two positive charges at two entrances and one negative charge between them with the opposite charge distribution on the other side. The overall view of the channels is as below (left image).





As one sees in above figure (right ones) , the number of permeation increases with temperature which is consistent with the Arrhenius relation. There is also, an abrupt jump in the number of permeation. But, as it can be seen, the jump temperature (*Tj*) which belongs to each system is different. As you see, the abrupt change in model 2, which is higher in number of permeation, has the highest *Tj* and The model 1, which has the less number of permeations, has the lowest *Tj*. It means that for each system, the more number of permeations leads to a higher *Tj*.
Such phenomena can be explained on the basis of the Arrhenius relation and the energy profile in the channel. This result shows that the Tj is porportional to the decrease or increase in hopping energy barrier for such systems.

Conclusion:
Investigation of the dynamic properties though the nanopores could help finding the better applications as well as increasing the efficiency of such processes. The single file permeation through the nanochannels will be increased with temperature and there will be a jump in the permeation. This temperature jump is related to the number of permeations and for a higher temperature, the jumping temperature will be higher.

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